Supplementary Material

**Supplementary table 1**

**1A: Metabolite list for bile acids (BAs)**

*#* **Metabolite Abbreviation BA class HMDB# Ion*a* Normalized to**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *1*  | Tauroursodeoxycholic acid  | TUDCA  | Taurine-conjugated  | HMDB0000874  | [M-H]  | TCA-*d*4  |
| *2*  | Taurocholic acid  | TCA  | Taurine-conjugated  | HMDB0000036  | [M-H]  | TCA-*d*4  |
| *3*  | Glycoursodeoxycholic acid  | GUDCA  | Glycine-conjugated  | HMDB0000708  | [M-H]  | TCA-*d*4  |
| *4* *5* *6* *7* *8* *9* *10* *11* *12* *13* *14* *15* *16* *17* *18*  | Glycocholic acid  | GCA  | Glycine-conjugated  | HMDB0000138  | [M-H]  | TDCA-*d*4  |
| Taurochenodesoxycholic acid  | TCDCA  | Taurine-conjugated  | HMDB0000951  | [M-H]  | TDCA-*d*4  |
| Taurodeoxycholic acid  | TDCA  | Taurine-conjugated  | HMDB0000896  | [M-H]  | TDCA-*d*4  |
| Sulfolithocholylglycine acid  | sGLCA  | Glycine-conjugated & sulfated  | HMDB0002639  | [M-H]  | CA-*d*5  |
| Cholic acid  | CA  | BA  | HMDB0000619  | [M+FA-H]  | CA-*d*5  |
| Ursodeoxycholic acid  | UDCA  | BA  | HMDB0000946  | [M+FA-H]  | CA-*d*5  |
| Hyodeoxycholic acid  | HDCA  | BA  | HMDB0000733  | [M-H]  | CA-*d*5  |
| Glycochenodeoxycholic acid  | GCDCA  | Glycine-conjugated  | HMDB0000637  | [M-H]  | CA-*d*5  |
| Glycodeoxycholic acid  | GDCA  | Glycine-conjugated  | HMDB0000631  | [M-H]  | CA-*d*5  |
| Chenodeoxycholic acid  | CDCA  | BA  | HMDB0000518  | [M+FA-H]  | CA-*d*5  |
| Deoxycholic acid  | DCA  | BA  | HMDB0000626  | [M-H]  | CA-*d*5  |
| Isolithocholic acid  | IsoLCA  | BA  | HMDB0000717  | [M-H]  | LCA-*d*5  |
| Lithocholic acid  | LCA  | BA  | HMDB0000761  | [M-H]  | LCA-*d*5  |
| Deoxycholic acid 3-sulfate  | sDCA  | Sulfated  | HMDB0002504  | [M-H]  | CA-*d*5  |
| Glycolithocholic acid  | GLCA  | Glycine-conjugated  | HMDB0000698  | [M-H]  | LCA-*d*5  |
| *19*  | Hyocholic acid  | HCA  | BA  | HMDB0000760  | [M+FA-H]  | TDCA-*d*4  |
| *20* *21* *22*  | 3-Oxocholic acid  | 3OCA  | BA  | HMDB0000502  | [M-H]  | CA-*d*5  |
| Chenodeoxycholic acid 3-sulfate  | sCDCA  | Sulfated  | HMDB0002586  | [M-H]  | CA-*d*5  |
| Lithocholic acid 3-sulfate  | sLCA  | Sulfated  | HMDB0000907  | [M-H]  | CA-*d*5  |

*a*Ion used in MS1 analysis.

**1B: Metabolite list for short-chain fatty acids (SCFAs)**

*#* **Metabolite Abbreviation SCFA class HMDB# Ion Normalized to**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| *1*  | Acetic acid  | Ace  | SCFA  |  | HMDB0000042  | [M-H]  | Acetic acid-13C2  |
| *2* *3*  | Propionic acid  | Prop  | SCFA  |  | HMDB0000237  | [M-H]  | Propionic acid-13C3  |
| Butyric acid  | But  | SCFA  |  | HMDB0000039  | [M-H]  | Butyric acid-13C4  |
| *4*  | Isobutyric acid  | iBut  | SCFA  |  | HMDB0001873  | [M-H]  | Butyric acid-13C4  |
| *5* *6* *7* *8* *9* *10* *11* *12* *13* *14* *15* *16* *17* *18* *19* *20*  | 2-Methylbutyric acid  | 2MeBut  | SCFA  |  | HMDB0002176  | [M-H]  | Butyric acid-13C4  |
| Valeric acid  | Val  | SCFA  |  | HMDB0000892  | [M-H]  | Butyric acid-13C4  |
| Isovaleric acid  | iVal  | SCFA  |  | HMDB0000718  | [M-H]  | Butyric acid-13C4  |
| Isocaproic acid  | iCap  | SCFA  |  | HMDB0000689  | [M-H]  | Butyric acid-13C4  |
| Caproic acid  | Cap  | SCFA  |  | HMDB0000535  | [M-H]  | Butyric acid-13C4  |
| D-Glyceric acid  | Glyceric  | SCFA-OH  |  | HMDB0000139  | [M-H]  | Acetic acid-13C2  |
| Glycolic acid  | Glyco  | SCFA-OH  |  | HMDB0000115  | [M-H]  | Acetic acid-13C2  |
| 3-Hydroxypropionic acid  | 3HPro  | SCFA-OH  |  | HMDB0000700  | [M-H]  | Acetic acid-13C2  |
| L-Lactic acid  | L-Lact  | SCFA-OH  |  | HMDB0000190  | [M-H]  | Acetic acid-13C2  |
| 3-Hydroxybutyric acid  | 3HBut  | SCFA-OH  |  | HMDB0000011  | [M-H]  | Acetic acid-13C2  |
| 2-Hydroxybutyric acid  | 2HBut  | SCFA-OH  |  | HMDB0000008  | [M-H]  | Propionic acid-13C3  |
| D/L-Malic acid  | Malic  | Dicarboxyl  |  | HMDB0031518/HMDB0000156  | [M-H]  | Butyric acid-13C4  |
| Malonic acid  | Malon  | Dicarboxyl  |  | HMDB0000691  | [M-H]  | Butyric acid-13C4  |
| Succinic acid  | Succin  | Dicarboxyl  |  | HMDB0000254  | [M-H]  | Butyric acid-13C4  |
| Glutaric acid  | Glutar  | Dicarboxyl  |  | HMDB0000661  | [M-H]  | Butyric acid-13C4  |
| Fumaric acid  | Fumar  | Dicarboxyl  |  | HMDB0000134  | [M-H]  | Butyric acid-13C4  |

**1C: Metabolite list amino acids (AAs)**

*#* **MetaboliteAbbreviationAA classHMDB#IonNormalized to**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *1*  | Pyroglutamic acid  | Glp  | α amino acids and derivatives  | HMDB0000267  | [M+H]  | Phenyl-13C6-alanine  |
| *2* *3*  | Phenylalanine  | Phe  | Phenylalanine and derivatives  | HMDB0000159  | [M+H]  | Phenyl-13C6-alanine  |
| Tryptophan  | Trp  | Indolyl carboxylic acids and derivatives  | HMDB0000929  | [M+H]  | Phenyl-13C6-alanine  |
| *4*  | Leucine  | Leu  | Leucine and derivatives  | HMDB0000687  | [M+H]  | Leucine-13C6,15N  |
| *5* *6* *7* *8* *9* *10* *11* *12* *13* *14* *15* *16* *17* *18* *19* *20*  | Isoleucine  | Ile  | Isoleucine and derivatives  | HMDB0000172  | [M+H]  | Isoleucine-13C6,15N  |
| Creatinine  | Cr  | α amino acids and derivatives  | HMDB0000562  | [M+H]  | Methionine-13C5,15N  |
| Methionine  | Met  | Methionine and derivatives  | HMDB0000696  | [M+H]  | Methionine-13C5,15N  |
| Tyrosine  | Tyr  | Tyrosine and derivatives  | HMDB0000158  | [M+H]  | Tyrosine-(phenyl-13C6)  |
| Proline  | Pro  | Proline and derivatives  | HMDB0000162  | [M+H]  | Proline-13C5  |
| Valine  | Val  | Valine and derivatives  | HMDB0000883  | [M+H]  | Valine-13C5  |
| α-Aminobutyric acid  | Abu  | L-α-amino acids  | HMDB0000452  | [M+H]  | Proline-13C5  |
| Glutamic Acid  | Glu  | Glutamic acid and derivatives  | HMDB0000148  | [M+H]  | Glutamic acid-13C5  |
| Threonine  | Thr  | L-α-amino acids  | HMDB0000167  | [M+H]  | Threonine-13C4  |
| Glutamine  | Gln  | L-α-amino acids  | HMDB0000641  | [M+H]  | Cystine-13C6,15N2  |
| Serine  | Ser  | Serine and derivatives  | HMDB0000187  | [M+H]  | Cystine-13C6,15N2  |
| 5-Aminopentanoic acid  | 5Ava  | Δ amino acids and derivatives  | HMDB0003355  | [M+H]  | Cystine-13C6,15N2  |
| Citrulline  | Cit  | L-α-amino acids  | HMDB0000904  | [M+H]  | Cystine-13C6,15N2  |
| Cystine  | Cys2  | L-cysteine-S-conjugates  | HMDB0000192  | [M+H]  | Cystine-13C6,15N2  |
| Asymmetric dimethylarginine  | ADMA  | Arginine and derivatives  | HMDB0001539  | [M+H]  | Histidine-13C6  |
| Histidine  | His  | Histidine and derivatives  | HMDB0000177  | [M+H]  | Histidine-13C6  |
| *21*  | 3-Methylhistidine  | 3MH  | Histidine and derivatives  | HMDB0000479  | [M+H]  | Histidine-13C6  |
| *22* *23* *24*  | Lysine  | Lys  | L-α-amino acids  | HMDB0000182  | [M+H]  | Lysine-13C6  |
| Ornithine  | Orn  | L-α-amino acids  | HMDB0000214  | [M+H]  | Lysine-13C6  |
| Arginine  | Arg  | L-α-amino acids  | HMDB0000517   | [M+H]  | Arginine-13C6  |